Internal One-Particle Density Matrix for Bose-Einstein Condensates with Finite Number of Particles in a Harmonic Potential

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Abstract

Investigations on the internal one-particle density matrix in the case of Bose-Einstein condensates with a finite number (N) of particles in a harmonic potential are performed. We solve the eigenvalue problem of the Pethick-Pitaevskii-type internal density matrix and find a fragmented condensate. On the contrary the condensate Jacobi-type internal density matrix gives complete condensation into a single state. The internal one-particle density matrix is, therefore, shown to be different in general for different choices of the internal coordinate system. We propose two physically motivated criteria for the choice of the adequate coordinate systems which give us a unique answer for the internal one-particle density matrix. One criterion is that in the infinite particle number limit ($N = \infty$) the internal one-particle density matrix should have the same eigenvalues and eigenfunctions as those of the corresponding ideal Bose-Einstein condensate in the laboratory frame. The other criterion is that the coordinate of the internal one-particle density matrix should be orthogonal to the remaining $(N-2)$ internal coordinates, though the $(N-2)$ coordinates, in general, do not need to be mutually orthogonal. This second criterion is shown to imply the first criterion. It is shown that the internal Jacobi coordinate system satisfies these two criteria while the internal coordinate system adopted by Pethick and Pitaevskii for the construction of the internal one-particle density matrix does not. It is demonstrated that these two criteria uniquely determine the internal one-particle density matrix which is identical to that calculated with the Jacobi coordinates. The relevance of this work concerning α-particle condensates in nuclei, as well as bosonic atoms in traps, is pointed out.

I. INTRODUCTION

The second 0^+ state of ^{12}C which is located near the 3α breakup threshold and is called the Hoyle state [1] is well known as one of the mysterious 0^+ states in light nuclei. The understanding of its structure has been actually one of the most difficult and challenging problems of nuclear structure. Its small excitation energy of 7.66 MeV is clearly not easy to explain by the shell model and, in fact, even the most advanced modern shell model approach known as the no-core shell model, fails by far to reproduce its position [2].

About 40 years ago Morinaga proposed to assign the 3α linear-chain structure to this Hoyle state [3]. However the observed reduced α decay width of this state which is larger than the Wigner limit value was pointed out to be contradictory to the linear-chain structure which can give at most only one third of the Wigner limit value [4]. The large α-decay reduced width of the Hoyle state in the ^{8}Be(0_1^+)+α channel was reproduced by a full three-body calculation with a semi-microscopic α-α interaction [5], namely an OCM (orthogonality condition model) [6] calculation for the 3α system. This 3α calculation contradicted the 3α chain structure of the Hoyle state and gave as the dominant component of the Hoyle state the ^{8}Be(0_1^+) + α structure with relative S wave between ^{8}Be(0_1^+) and α. Since ^{8}Be(0_1^+) consists of two α clusters weakly coupled in relative S wave, the Hoyle state was concluded to have a weakly coupled 3α structure in relative S waves with large spatial extent, which is a gas-like structure of α clusters. A few years later, this understanding of the structure of the Hoyle state was reported to be reproduced by full microscopic 3α calculations by two groups, namely Kamimura and his collaborators [7] and Uegaki and his collaborators [8]. These calculations nicely reproduced not only the position of the Hoyle state but also other experimental properties including inelastic electron form factor and E0 and E2 transition properties. Other states of ^{12}C below and around the Hoyle state were also well described. The microscopic 3α model treatments of ^{12}C of Refs. [7, 8] were later extended to reaction theory in Ref. [9]. Furthermore investigation by antisymmetrized molecular dynamics [10] and that by fermionic molecular dynamics [11] starting from a realistic bare N-N force, both of which do not assume alpha clustering, have now reproduced all the salient features of the Hoyle state [1]. Let us also mention that for a product state of only a few bosons, the phase fluctuates. However, we use the word 'condensate' in the same 'loose' sense as nuclear physicists are used to say that 'nuclei are superfluid', in spite of the fact that there

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is not a macroscopic number of Cooper pairs in nucleus.

Almost 30 years after the first proposal of the $^8\text{Be}(0^+_1) + \alpha$ structure for the Hoyle state, this state was reconsidered in a new light in Ref. [12] involving four members of the present authors. They presented the following new model wave function $\Phi_B(3\alpha)$, called the THSR wave function:

$$\Phi_B(3\alpha) = \mathcal{A}\{\exp[-\frac{2}{B^2}(\boldsymbol{X}_1^2 + \boldsymbol{X}_2^2 + \boldsymbol{X}_3^2)] \ \phi(\alpha_1)\phi(\alpha_2)\phi(\alpha_3)\} \tag{1}$$

$$= \exp(-\frac{6}{B^2}\boldsymbol{\xi}_3^2)\mathcal{A}\{\exp(-\frac{4}{3B^2}\boldsymbol{\xi}_1^2 - \frac{1}{B^2}\boldsymbol{\xi}_2^2) \ \phi(\alpha_1)\phi(\alpha_2)\phi(\alpha_3)\}, \tag{2}$$

$$\boldsymbol{\xi}_1 = \boldsymbol{X}_1 - \frac{1}{2}(\boldsymbol{X}_2 + \boldsymbol{X}_3), \ \boldsymbol{\xi}_2 = \boldsymbol{X}_2 - \boldsymbol{X}_3, \ \boldsymbol{\xi}_3 = \frac{1}{3}(\boldsymbol{X}_1 + \boldsymbol{X}_2 + \boldsymbol{X}_3), \tag{3}$$

where $\phi(\alpha_j)$ and $\boldsymbol{X}_j$ stand for the internal wave function and the center-of-mass coordinate of the j-th α cluster, respectively, and $\mathcal{A}$ is the antisymmetrizer of the nucleons. As shown in Eq. (2), the THSR wave function can be regarded as expressing the cluster structure where a $^8\text{Be}(0^+_1)$-like cluster $\mathcal{A}\{\exp(-(1/B^2)\boldsymbol{\xi}_2^2)\phi(\alpha_2)\phi(\alpha_3)\}$ and the α_1 cluster couple via an S-wave inter-cluster wave function $\exp(-(4/3B^2)\boldsymbol{\xi}_1^2)$. On the other hand, Equation (1) shows that the THSR wave function represents the state where three α clusters occupy the same single $0S$-orbit $\exp(-(2/B^2)\boldsymbol{X}^2)$, namely a 3α condensate state which is the finite size counterpart of the macroscopic α-particle condensation in infinite nuclear matter at low density [13]. What the authors of Ref. [12] proposed was that the $^8\text{Be}(0^+_1) + \alpha$ structure of the Hoyle state can be regarded as being a 3α condensate state and that one can expect in general the existence of $n\alpha$ condensate states in the vicinity of the $n\alpha$ breakup threshold in $4n$ self-conjugate nuclei [14]. It was soon discovered [15] that the microscopic 3α wave functions of both of Refs. [7, 8] have overlaps of more than 95% with a single THSR wave function with a large size parameter B, implying small overlaps between individual α clusters.

This above-mentioned striking fact reported in Ref. [15] means without doubt that the Hoyle state structure has a strong relation with the α condensation physics in dilute infinite nuclear matter. One of the important tasks for the clarification of this relation is to study the magnitude of the component of the ideal Bose-Einstein condensation of structureless α particles which is contained in the Hoyle state wave function. This was investigated by the authors of Refs. [16, 17] who solved the eigenvalue problem of the internal one-particle density matrix of the Hoyle state wave functions where the center-of-mass coordinate is eliminated. As the internal coordinates for calculating the internal one-particle density matrix ρ they used the Jacobi coordinates, namely $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ in Eq. (3). They obtained a

maximum eigenvalue larger than 0.7 for the normalized density matrix ρ (Tr $\rho = 1$), which means that the corresponding eigenfunction which is a $0S$-orbit is occupied to more than 70% by the three α particles. This is a large percentage corroborating the almost ideal α-particle condensation nature of the Hoyle state, that is the Hoyle state is describable to very good approximation by a product state of these bosons, each in the same $0S$ orbit [16, 17].

For the discussion of the Bose-Einstein condensation of a confined macroscopic system, one uses in general the one-particle density matrix in the laboratory frame where the coordinate system consisting of individual particle coordinates is adopted. However, Pethick and Pitaevskii [18] (PP) proposed to use the internal one-particle density matrix by eliminating the center-of-mass coordinate when one discusses the condensate fraction of the system where only the center-of-mass degree of freedom is excited but all relative degrees of freedom are kept unchanged. Their proposal was to point out that the conclusion of the paper by Wilkin et al. [19] does not appropriately reflect the physics. Wilkin et al. discussed the lowest excitation of a condensate of cold bosonic atoms with attractive interactions which rotates with its center of mass in a harmonic potential but keeps all the internal degrees of freedom as in its ground state which shows complete condensation. It was found that the corresponding one-body density matrix in the laboratory frame has many eigenvalues of comparable size, and thus the system should be characterized as a fragmented condensate [19]. On the other hand PP claimed that if one uses an internal one-particle density matrix by eliminating the center-of-mass coordinate it should give a single eigenvalue of the order of the number of particles indicating the non-fragmented condensate character of the internal part of the system. Unfortunately PP presented only their idea and did not demonstrate explicit results of the diagonalization of their definition of the internal one-particle density matrix.

In this paper, following the definition of PP, we construct the internal one-particle density matrix of a many-boson system in a harmonic trap and then give the explicit analytical form of the eigenvalues and eigenfunctions of this density matrix. We will see that the eigenvalues are fragmented, which is contrary to PP's initial objective. We will discuss that this result does not mean that the original idea of PP is incorrect but it means that the internal coordinate system which PP adopted is inadequate. Actually when we construct the internal one-particle density matrix by using the internal Jacobi coordinates, the resulting eigenvalues show complete condensation. We will give two criteria for the choice of the

adequate coordinate systems which will give us a unique answer for the definition of the internal one-particle density matrix. One criterion is that in the infinite particle number limit ($N = \infty$) the internal one-particle density matrix should have the same eigenvalues and eigenfunctions as those of the corresponding ideal Bose-Einstein condensate in the laboratory frame. This is in line with the general wisdom that in the thermodynamic limit all macroscopic quantities shall be the same, regardless whether considered in the laboratory frame or in the internal frame [20]. The other criterion is that the coordinate used in the internal one-particle density matrix should be orthogonal to (or maximally independent from) the remaining $(N - 2)$ internal coordinates, though the $(N - 2)$ coordinates, in general, do not need to be mutually orthogonal. This second criterion is shown to imply the first criterion. We show that the internal Jacobi coordinate system satisfies these two criteria, while the internal coordinate system adopted by PP for the construction of the internal one-particle density matrix does not. Furthermore we argue that these two criteria uniquely determine the internal one-particle density matrix which is the same as that calculated with the Jacobi coordinates. The results of this paper justify the use of the Jacobi coordinates in Refs. [16, 17] and, hence, corroborate the almost ideal α-particle condensation nature of the Hoyle state.

The present paper is organized as follows. In Sec. II, we formulate the internal one-particle density matrix with respect to the internal wave function of a Bose-Einstein condensate with finite particle number in a harmonic trap. Then, the analytical form of the eigenvalues and eigenfunctions is presented for the internal density matrix and numerical eigenvalues are discussed. In Sec. III. we propose two criteria for the choice of proper coordinate systems for internal one-particle density matrix. Finally, the summary is given in Sec. IV. Appendix A serves to present the analytical solution of the eigenvalue problem of the density matrix and Appendix B is given for the explanation of the bosonic symmetry of the Jacobi-type internal one-particle density matrix. The original version of this paper was given in an article on the arXiv [21] and a short version of this paper is reported in a letter paper [22] with special attention to the cold atom community.

II. INTERNAL ONE-PARTICLE DENSITY MATRIX

First we consider the one-particle density matrix in the laboratory frame for an ideal Bose-Einstein condensate with N spinless bosons in a harmonic potential. The result is trivial but instructive for studying the nature of the internal one-particle density matrix, as will be discussed later.

The N-particle Hamiltonian in laboratory frame is presented as

$$H = \sum_{i=1}^{N} \frac{1}{2m} \boldsymbol{p}_i^2 + \sum_{i=1}^{N} \frac{1}{2} m\omega^2 \boldsymbol{r}_i^2. \tag{4}$$

The normalized ground-state wave function of this system is expressed as a product of identical Gaussian single-particle wave functions, i.e.

$$\Phi(\{\boldsymbol{r}_i\}_{i=1}^{N}) = \prod_{i=1}^{N} \left(\frac{2\nu}{\pi}\right)^{3/4} \exp\left(-\nu \boldsymbol{r}_i^2\right) \tag{5}$$

$$= \left(\frac{2\nu}{\pi}\right)^{3N/4} \exp\left(-\nu \sum_{i=1}^{N} \boldsymbol{r}_i^2\right) \tag{6}$$

where $\nu = m\omega/2\hbar$, and $\{\boldsymbol{r}_i\}_{i=1}^{N}$ denotes the set of the coordinates $\boldsymbol{r}_i$ $(i = 1 \cdots, N)$. The one particle density matrix in the laboratory frame is defined as

$$\rho_{\text{Lab}}^{(1)}(\boldsymbol{r}, \boldsymbol{r}') = \int d\boldsymbol{r}_2 d\boldsymbol{r}_3 \cdots d\boldsymbol{r}_N \Phi^*(\boldsymbol{r}, \boldsymbol{r}_2, \boldsymbol{r}_3, \cdots, \boldsymbol{r}_N) \Phi(\boldsymbol{r}', \boldsymbol{r}_2, \boldsymbol{r}_3, \cdots, \boldsymbol{r}_N), \tag{7}$$

$$= \left(\frac{2\nu}{\pi}\right)^{3/2} \exp\left[-\nu(\boldsymbol{r}^2 + \boldsymbol{r}'^2)\right]. \tag{8}$$

It is noted that the density matrix is independent of the number of particles N and is separable with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$. The separability originates from the fact that the Hamiltonian is separable with respect to different particle operators, $\boldsymbol{r}_i$ and $\boldsymbol{p}_i$ $(i = 1, \cdots, N)$, in Eq. (4), or equivalently from the fact that the wave function of Eq. (6) is separable with respect to different particle coordinates, $\boldsymbol{r}_i$ $(i = 1, \cdots, N)$.

The nature of the single particle orbits and their occupation probabilities in the relevant system can be obtained by solving the eigenvalue problem of the density matrix,

$$\int \rho_{\text{Lab}}^{(1)}(\boldsymbol{r}, \boldsymbol{r}') \phi(\boldsymbol{r}') d\boldsymbol{r}' = \lambda \phi(\boldsymbol{r}), \tag{9}$$

where $\phi(\boldsymbol{r})$ is the single particle orbit, and λ is its occupation probability. This equation can easily be solved, and we find that the density matrix has only one non zero eigenvalue $\lambda = 1$ with one eigenfunction, namely, the zero-node S-wave Gaussian $\phi(\boldsymbol{r}) = (2\nu/\pi)^{3/4} \exp(-\nu \boldsymbol{r}^2)$

(or $0S$ harmonic oscillator wave function $\phi_{000}(\boldsymbol{r}, \nu)$, which will be defined later) with 100 % occupancy ($\lambda = 1$). This means that all particles are condensed in that single orbit, i.e. an ideal Bose-Einstein condensation is realized in the laboratory frame. This feature is independent of the number of particles N.

Next we consider the internal one-particle density matrix for the N-particle Bose-Einstein condensation in a harmonic trap described by the wave function Eq. (6) with the total Hamiltonian Eq. (4). *Internal* means that the density is free from the center-of-mass coordinate of the system, as it must be the case, when dealing with, e.g., selfbound systems. In the present paper, two kinds of internal coordinate sets are introduced; 1) coordinates with respect to the center of mass of the total system and 2) Jacobi coordinates. The former set was first considered by Pethick and Pitaevskii [18] to define the internal one-particle density matrix. We call it Pethick-Pitaevskii-type (PP-type) internal one-particle density matrix in the present paper. For the latter set, we call it Jacobi-type density matrix.

A. Pethick-Pitaevskii-type internal one-particle density matrix

As already mentioned in the introduction, Pethick and Pitaevskii proposed to consider the internal single particle density matrix for a Bose condensed system when only the center-of-mass but no internal degree of freedom is excited. In order to define an internal one-particle density matrix, Pethick and Pitaevskii adopted internal coordinates defined with respect to the center of mass of the total system [18]. The center-of-mass coordinate $\boldsymbol{R}$ and the coordinate $\boldsymbol{q}_i$ of particle i relative to the center of mass are given, respectively, by

$$\boldsymbol{R} = \frac{1}{N} \sum_{i=1}^{N} \boldsymbol{r}_i, \quad \boldsymbol{q}_i = \boldsymbol{r}_i - \boldsymbol{R}. \tag{10}$$

Since $\sum_{i=1}^{N} \boldsymbol{q}_i = 0$, only $N-1$ of the $\boldsymbol{q}_i$ are independent. Hereafter, as the independent internal coordinates, we adopt $\boldsymbol{q}_i$ ($i = 1, \cdots, N-1$). We introduce the conjugate momenta $\boldsymbol{\pi}_i$ ($i = 1, \cdots, N-1$) and $\boldsymbol{P}$ for the coordinates $\boldsymbol{q}_i$ ($i = 1, \cdots, N-1$) and $\boldsymbol{R}$, respectively. Then, the total Hamiltonian in Eq. (4) is rewritten as

$$H = H_{\text{int}} + H_{\text{cm}}, \tag{11}$$

$$H_{\text{int}} = \frac{1}{2m} \left[\left(\frac{N-1}{N} \right) \sum_{i=1}^{N-1} \boldsymbol{\pi}_i^2 - \frac{2}{N} \sum_{i<i'=1}^{N-1} \boldsymbol{\pi}_i \cdot \boldsymbol{\pi}_{i'} \right] + m\omega^2 \left[\sum_{i=1}^{N-1} \boldsymbol{q}_i^2 + \sum_{i<i'=1}^{N-1} \boldsymbol{q}_i \cdot \boldsymbol{q}_{i'} \right], \tag{12}$$

$$H_{\text{cm}} = \frac{1}{2Nm} \boldsymbol{P}^2 + \frac{1}{2} Nm\omega^2 \boldsymbol{R}^2, \tag{13}$$

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where H_{int} and H_{cm} denote the internal and center-of-mass Hamiltonians, respectively. It should be mentioned that the above Hamiltonian includes the cross terms, $\boldsymbol{q}_i \cdot \boldsymbol{q}_{i'}$ and $\boldsymbol{\pi}_i \cdot \boldsymbol{\pi}_{i'}$, which, in general, appear so far as one takes non-orthonormal coordinate systems [23–26].

By using the relation

$$\sum_{i=1}^{N} \boldsymbol{r}_i^2 = N\boldsymbol{R}^2 + \sum_{i,i'=1}^{N-1} (\delta_{i,i'} + 1)\boldsymbol{q}_i \cdot \boldsymbol{q}_{i'}, \tag{14}$$

the total wave function in Eq. (6) is expressed as

$$\Phi(\{\boldsymbol{r}_i\}_{i=1}^{N}) = \frac{1}{N^{3/2}} \times \Phi_{\text{int}}(\{\boldsymbol{q}_i\}_{i=1}^{N-1})\Phi_{\text{cm}}(\boldsymbol{R}), \tag{15}$$

$$\Phi_{\text{int}}(\{\boldsymbol{q}_i\}_{i=1}^{N-1}) = \left(\frac{N \times (2\nu)^{N-1}}{\pi^{N-1}}\right)^{3/4} \exp\left[-\sum_{i,i'=1}^{N-1} (\delta_{ii'} + 1)\nu\boldsymbol{q}_i \cdot \boldsymbol{q}_{i'}\right], \tag{16}$$

$$\Phi_{\text{cm}}(\boldsymbol{R}) = \left(\frac{2N\nu}{\pi}\right)^{3/4} \exp(-N\nu\boldsymbol{R}^2), \tag{17}$$

where Φ_{int} and Φ_{cm} denote the internal and center-of-mass wave functions, respectively. The separability of Φ_{int} and Φ_{cm} comes from the fact that the total Hamiltonian is separable with respect to the internal and center-of-mass parts [see Eq. (11)] or directly from Eq. (14) inserted into Eq. (6). The factor $1/N^{3/2}$ in Eq. (15) drops out when taking into account the Jacobian $\partial(\{\boldsymbol{r}_i\}_{i=1}^{N})/\partial(\{\boldsymbol{q}_i\}_{i=1}^{N-1}, \boldsymbol{R}) = N^3$, coming from the coordinate transformation from the space-fixed system to the center-of-mass system. It should be noted that both wave functions Φ_{int} and Φ_{cm} are normalized and satisfy $H_{\text{int}}\Phi_{\text{int}} = (3/2)(N-1)\hbar\omega\Phi_{\text{int}}$ and $H_{\text{cm}}\Phi_{\text{cm}} = (3/2)\hbar\omega\Phi_{\text{cm}}$, respectively.

According to Pethick and Pitaevskii [18], the internal one-particle density matrix is defined as,

$$\rho_{\text{int,PP}}^{(1)}(\boldsymbol{q}, \boldsymbol{q}') = \int d\boldsymbol{q}_2 \cdots d\boldsymbol{q}_{N-1} \, \rho_{\text{int,PP}}(\boldsymbol{q}, \boldsymbol{q}_2, \cdots, \boldsymbol{q}_{N-1}; \boldsymbol{q}', \boldsymbol{q}_2, \cdots, \boldsymbol{q}_{N-1}), \tag{18}$$

$$\rho_{\text{int,PP}}(\{\boldsymbol{q}_i\}_{i=1}^{N-1}, \{\boldsymbol{q}_i'\}_{i=1}^{N-1}) = N^3 \int d\boldsymbol{R} \, \Phi^*(\{\boldsymbol{q}_i + \boldsymbol{R}\}_{i=1}^{N})\Phi(\{\boldsymbol{q}_i' + \boldsymbol{R}\}_{i=1}^{N}), \tag{19}$$

where the Jacobian factor N^3 is inserted in the above equation, which is missing in Ref. [18]. Using the wave function $\Phi(\{\boldsymbol{r}_i\}_{i=1}^{N})$ in Eq. (6), the internal one-particle density matrix (18) is expressed as

$$\rho_{\text{int,PP}}^{(1)}(\boldsymbol{q}, \boldsymbol{q}') = \left(\frac{N}{N-1}\right)^{3/2}\left(\frac{2\nu}{\pi}\right)^{3/2} \exp\left[-\frac{3N-2}{2(N-1)}\nu(\boldsymbol{q}^2 + \boldsymbol{q}'^2) + \frac{N-2}{N-1}\nu\boldsymbol{q} \cdot \boldsymbol{q}'\right]. \tag{20}$$

It is noted that this density matrix depends on the number of particles N and contains the cross term $\boldsymbol{q} \cdot \boldsymbol{q}'$. The origin of the cross term comes from the nonseparability of the

coordinate $\boldsymbol{q}_1$ from the other $(N-2)$ coordinates $\boldsymbol{q}_i$ $(i = 2, \cdots, N-1)$ in the internal wave function of Eq. (16), or equivalently from the fact that the internal Hamiltonian of Eq. (12) is non-separable between the first particle operators $\boldsymbol{\pi}_1$ and $\boldsymbol{q}_1$ and the other $(N-2)$ particle operators $\boldsymbol{\pi}_i$ and $\boldsymbol{q}_i$ $(i = 2, \cdots, N-1)$. The result of Eq. (20) can also be verified with the use of the internal density matrix in Eq. (19) presented as follows:

$$\rho_{\text{int,PP}}(\{\boldsymbol{q}_i\}_{i=1}^{N-1}, \{\boldsymbol{q}_i'\}_{i=1}^{N-1}) = \Phi_{\text{int}}^*(\{\boldsymbol{q}_i\}_{i=1}^{N-1})\Phi_{\text{int}}(\{\boldsymbol{q}_i'\}_{i=1}^{N-1}), \tag{21}$$

where $\Phi_{\text{int}}^*(\{\boldsymbol{q}_i\}_{i=1}^{N-1})$ is the internal wave function defined in Eq. (16).

Let us discuss the nature of the internal one-particle density $\rho_{\text{int}}^{(1)}(\boldsymbol{q}, \boldsymbol{q}')$. First we study the single-particle orbits and their eigenvalues obtained by solving the eigenvalue problem for the density matrix,

$$\int \rho_{\text{int,PP}}^{(1)}(\boldsymbol{q}, \boldsymbol{q}')\phi(\boldsymbol{q})d\boldsymbol{q}' = \lambda\phi(\boldsymbol{q}). \tag{22}$$

This equation can be solved analytically. There are several ways to solve it. In Appendix A we give one method. We can also analyze the description given in Ref. [27]. The single-particle orbits ϕ are expressed by the harmonic oscillator wave functions $\phi_{nLM}(\boldsymbol{q}, \beta_N)$ with the orbital angular momentum L, magnetic quantum number M and harmonic oscillator quanta $Q = 2n + L$ $(n = 0, 1, 2, \cdots)$,

$$\phi_{nLM}(\boldsymbol{q}, \beta_N) = \left[\frac{(2\beta_N)^{L+3/2}2^{n+L+2}n!}{\sqrt{\pi}(2n + 2L + 1)!!}\right]^{1/2} q^L L_n^{(L+1/2)}(2\beta_N q^2)\exp(-\beta_N q^2)Y_{LM}(\hat{\boldsymbol{q}}), \tag{23}$$

$$\beta_N = \sqrt{\frac{2N}{N-1}}\nu. \tag{24}$$

The eigenvalues or occupation probabilities λ are given as

$$\lambda_{n,N}^{(LM)} = \left[\frac{4N}{3N - 2 + 2\sqrt{2N(N-1)}}\right]^{3/2} \left[\frac{N-2}{3N - 2 + 2\sqrt{2N(N-1)}}\right]^{2n+L}, \tag{25}$$

and satisfy the following completeness relation,

$$\sum_{L=0}^{\infty} \sum_{M=-L}^{L} \sum_{n=0}^{\infty} \lambda_{n,N}^{(LM)} = 1. \tag{26}$$

Then, the internal one-particle density matrix for the N particles in Eq. (20) can be presented in terms of the wave functions (23)

$$\rho_{\text{int,PP}}^{(1)}(\boldsymbol{q}, \boldsymbol{q}') = \sum_{L=0}^{\infty} \sum_{M=-L}^{L} \sum_{n=0}^{\infty} |\phi_{nLM}(\boldsymbol{q}, \beta_N)\rangle \, \lambda_{n,N}^{(LM)} \, \langle\phi_{nLM}(\boldsymbol{q}', \beta_N)|. \tag{27}$$

The occupation probability with respect to the partial wave with quantum number L is defined as

$$\Lambda_N^{(L)} = \sum_{M=-L}^{L} \sum_{n=0}^{\infty} \lambda_{n,N}^{(LM)}. \tag{28}$$

In the macroscopic limit $(N \to \infty)$, the internal one-particle density matrix $\rho_{\mathrm{int,PP},N=\infty}^{(1)}$, its eigenfunctions $\phi_{\mathrm{int,PP},N=\infty}$, and eigenvalues $\lambda_{n,N=\infty}^{(LM)}$ are given by

$$\rho_{\mathrm{int,PP},N=\infty}^{(1)}(\boldsymbol{q},\boldsymbol{q}') = \left(\frac{2\nu}{\pi}\right)^{3/2} \exp\left[-\frac{3}{2}\nu(\boldsymbol{q}^2 + \boldsymbol{q}'^2) + \nu\boldsymbol{q}\cdot\boldsymbol{q}'\right], \tag{29}$$

$$\phi_{\mathrm{int,PP},N=\infty}(\boldsymbol{q}) = \phi_{nLM}(\boldsymbol{q}, \sqrt{2}\nu), \tag{30}$$

$$\lambda_{n,N=\infty}^{(LM)} = 2^3(3 - 2\sqrt{2})^{2n+L+3/2}, \tag{31}$$

$$\Lambda_{N=\infty}^{(L)} = \sum_{M=-L}^{L} \sum_{n=0}^{\infty} \lambda_{n,N=\infty}^{(LM)} = (2L+1)(2-\sqrt{2})(3-2\sqrt{2})^L. \tag{32}$$

We remark that the summed eigenvalues $\Lambda_{N=\infty}^{(L)}$ still depend on the angular momentum L.

The eigenvalue or occupation probability of the PP-type internal one-particle density matrix, $\Lambda_N^{(L)}$ of Eq. (28) depends on the orbital angular momentum L, and the particle number N. In the case of $N = 3$, we obtain the occupation probabilities, $\Lambda_3^{(S)} = 0.804$ for S wave, $\Lambda_3^{(P)} = 0.173$ for P, $\Lambda_3^{(D)} = 0.021$ for D, $\Lambda_3^{(F)} = 0.002$ for F, and so on. Increasing the particle number, the S-wave occupation probability is decreasing, while the higher partial-wave ones are increasing (see Fig. 1 in Refs. [21, 22]). These results show that the PP-type one-particle density matrix leads to a fragmented condensate. The reason why the PP-type internal density matrix shows the fragmented condensate is due to the existence of the cross term $\boldsymbol{q}\cdot\boldsymbol{q}'$ in Eq. (20).

B. Jacobi-type internal one-particle density matrix

For the N-particle system, we define the $(N-1)$ internal Jacobi coordinates $\{\boldsymbol{\xi}_i, (i = 1,\cdots,N-1)\}$ and the center-of-mass coordinate $\boldsymbol{R}$ as follows:

$$\boldsymbol{\xi}_i = \boldsymbol{r}_i - \frac{1}{N-i}\sum_{k=i+1}^{N} \boldsymbol{r}_k, \quad \text{for } i = 1, 2, \cdots, N-1 \tag{33}$$

$$\boldsymbol{R} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{r}_i, \tag{34}$$

where $\boldsymbol{\xi}_1$ denotes the relative coordinate between the first particle and the remaining $(N-1)$ particles, and other Jacobi coordinates are self-evident. Then, the N-particle Hamiltonian in Eq. (4) can be separated into the internal and center-of-mass Hamiltonian,

$$H = H_{\text{int}} + H_{\text{cm}}, \tag{35}$$

$$H_{\text{int}} = \sum_{i=1}^{N-1}\{\frac{1}{2\mu_i}\boldsymbol{\pi}_i^2 + \frac{1}{2}\mu_i\omega^2\boldsymbol{\xi}_i^2\}, \quad \mu_i = \frac{N-i}{N-i+1}m, \tag{36}$$

$$H_{\text{cm}} = \frac{1}{2Nm}\boldsymbol{P}^2 + \frac{1}{2}Nm\omega^2\boldsymbol{R}^2, \tag{37}$$

where $\boldsymbol{\pi}_i$ and $\boldsymbol{P}$ denote the conjugate momenta corresponding to the coordinates $\boldsymbol{\xi}_i$ and $\boldsymbol{R}$, respectively.

Since the total Hamiltonian is a sum of decoupled N harmonic oscillator Hamiltonians (for $\boldsymbol{R}$ and $(N-1)$ internal Jacobi coordinates), the total wave function in Eq. (6) is expressed as

$$\Phi(\{\boldsymbol{r}_i\}_{i=1}^{N}) = \Phi_{\text{int}}(\{\boldsymbol{\xi}_i\}_{i=1}^{N-1})\Phi_{\text{cm}}(\boldsymbol{R}), \tag{38}$$

$$\Phi_{\text{int}}(\{\boldsymbol{\xi}_i\}_{i=1}^{N-1}) = \prod_{i=1}^{N-1}\left(\frac{2\nu_i}{\pi}\right)^{3/4}\exp\left(-\nu_i\boldsymbol{\xi}_i^2\right) \tag{39}$$

$$= \left(\frac{(2\nu)^{N-1}}{N\times\pi^{N-1}}\right)^{3/4}\exp\{-\sum_{i=1}^{N-1}\nu_i\boldsymbol{\xi}_i^2\}, \quad \nu_i = \frac{N-i}{N-i+1}\nu, \tag{40}$$

$$\Phi_{\text{cm}}(\boldsymbol{R}) = \left(\frac{2N\nu}{\pi}\right)^{3/4}\exp(-N\nu\boldsymbol{R}^2). \tag{41}$$

This expression of $\Phi(\{\boldsymbol{r}_i\}_{i=1}^{N})$ can also be derived by inserting the relation

$$\sum_{i=1}^{N}\boldsymbol{r}_i^2 = N\boldsymbol{R}^2 + \sum_{i=1}^{N-1}\frac{\nu_i}{\nu}\boldsymbol{\xi}_i^2, \tag{42}$$

into the original expression given in Eq. (6). The total wave function is the product of the internal and center-of-mass wave functions, Φ_{int} and Φ_{cm}, which are normalized and satisfy the relations, $H_{\text{int}}\Phi_{\text{int}} = (3/2)(N-1)\hbar\omega\Phi_{\text{int}}$ and $H_{\text{cm}}\Phi_{\text{cm}} = (3/2)\hbar\omega\Phi_{\text{cm}}$. It is noted that the internal wave function is given as a product of harmonic oscillator wave functions $\phi_{000}(\boldsymbol{\xi}_i, \nu_i)$ $(i = 1, \cdots, N-1)$.

The Jacobi-type internal density matrix writes

$$\rho_{\text{int,J}}(\{\boldsymbol{\xi}_i\}_{i=1}^{N-1}, \{\boldsymbol{\xi}_i'\}_{i=1}^{N-1}) = \Phi_{\text{int}}^*(\{\boldsymbol{\xi}_i\}_{i=1}^{N-1})\Phi_{\text{int}}(\{\boldsymbol{\xi}_i'\}_{i=1}^{N-1}). \tag{43}$$

Then, the Jacobi-type one-particle density matrix is defined with respect to $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_1'$ as

$$\rho_{\text{int,J}}^{(1)}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \int d\boldsymbol{\xi}_2\cdots d\boldsymbol{\xi}_{N-1}\,\rho_{\text{int,J}}(\boldsymbol{\xi}, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1}; \boldsymbol{\xi}', \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1}), \tag{44}$$

$$= \left(\frac{N-1}{N}\right)^{3/2} \left(\frac{2\nu}{\pi}\right)^{3/2} \exp\left[-\frac{N-1}{N}\nu(\boldsymbol{\xi}^2 + \boldsymbol{\xi}'^2)\right]. \tag{45}$$

This choice of the coordinate $\boldsymbol{\xi}_1$ for the internal density matrix is natural, because the single particle orbit should be defined with respect to the relative coordinate between one particle and the other remaining $N-1$ particles in the Jacobi coordinate system. The compatibility between the bosonic symmetry of the system and the above definition of the internal one-particle density matrix, where it may seem that one special coordinate is singled out, is explained in Appendix B. The eigenvalue equation of the one-particle density matrix can easily be solved analytically. We find that the density matrix has only one non-zero eigenvalue $\lambda = 1$ with corresponding eigenfunction $\phi_{\text{int,J},N}$ which is the $0S$ harmonic oscillator wave function with 100 % occupancy ($\lambda = 1$),

$$\phi_{\text{int,J},N}(\boldsymbol{\xi}) = \delta_{L0}\delta_{M0}\phi_{000}(\boldsymbol{\xi}, (N-1)\nu/N), \tag{46}$$

$$\lambda_N^{(LM)} = \delta_{L0}\delta_{M0}, \tag{47}$$

$$\Lambda_N^{(L)} = \sum_{M=-L}^{L} \lambda^{(LM)} = \delta_{L0}. \tag{48}$$

This means that all particles are condensed in the single $0S$ particle state, although the size parameter in the state [Eq. (46)] depends on N and is slightly different from that in the eigenfunction $\phi_{000}(\boldsymbol{r}, \nu)$ in laboratory frame, discussed in the beginning of Sec. II. In the macroscopic limit ($N \to \infty$), the internal one-particle density matrix $\rho^{(1)}_{\text{int,PP},N=\infty}$, its eigenfunction $\phi_{\text{int,PP},N=\infty}$, and eigenvalues $\lambda^{(LM)}_{n,N=\infty}$ are given by

$$\rho^{(1)}_{\text{int,J},N=\infty}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \left(\frac{2\nu}{\pi}\right)^{3/2} \exp\left[-\nu(\boldsymbol{\xi}^2 + \boldsymbol{\xi}'^2)\right], \tag{49}$$

$$\phi_{\text{int,J},N=\infty}(\boldsymbol{\xi}) = \delta_{L0}\delta_{M0}\phi_{000}(\boldsymbol{\xi}, \nu), \tag{50}$$

$$\lambda^{(LM)}_{N=\infty} = \delta_{L0}\delta_{M0}, \tag{51}$$

$$\Lambda^{(L)}_{N=\infty} = \sum_{M=-L}^{L} \lambda^{(LM)}_{N=\infty} = \delta_{L0}. \tag{52}$$

The Jacobi-type one-particle density matrix for finite particle number is separable with respect to the coordinates $\boldsymbol{\xi}$ and $\boldsymbol{\xi}'$. This leads to the only one non-zero eigenvalue $\lambda = 1$ which is the same as for an ideal Bose-Einstein condensate system in the laboratory system. Also the internal density matrix (49) becomes identical to the one in the laboratory system, Eq. (8), for $N = \infty$. The separability of the internal density matrix comes from the separability of the internal wave function in Eq. (40) with respect to different Jacobi

coordinates, which originates from the separability of the internal Hamiltonian in Eq. (36) with respect to different Jacobi coordinates. This feature has it origin in the fact that the Jacobi coordinates form an orthogonal coordinate system.

III. CRITERION FOR THE CHOICE OF ADEQUATE INTERNAL COORDINATES

A. Convergence to Bose-Einstein Condensation in the Macroscopic Limit

In the previous section we learned that the outcome of the diagonalization of the internal density matrix depends on the choice of the internal coordinates. This is a serious problem for treating condensates in internal self-bound systems such as α-particle condensates in nuclear systems or small droplets of superfluid ^{4}He, because only internal degrees of freedom are relevant in these systems.

In order to overcome the difficulty, we gave a criterion for the choice of the internal coordinates: In the macroscopic limit ($N \to \infty$) the internal density matrix should have the same eigenvalues and eigenfunctions as those of the ideal Bose-Einstein condensate in the laboratory frame. This is a very physical boundary condition. For understanding this physical condition, consideration of the following situation in the macroscopic limit may be helpful: In the laboratory frame, the center-of-mass motion of the present system is described by the wave function $\Phi_{\mathrm{cm}}(\boldsymbol{R})$ of Eq. (17). In the macroscopic limit, the center-of-mass coordinate should be at the coordinate origin of the laboratory frame, because the probability of finding the center-of-mass coordinate at position $\boldsymbol{R}$ is given by $|\Phi_{\mathrm{cm}}(\boldsymbol{R})|^2 = (2N\nu/\pi)^{3/2} \exp(-2N\nu\boldsymbol{R}^2)$ which becomes a delta function $\delta(\boldsymbol{R})$ in the limit of $N \to \infty$. Thus the internal coordinate $\boldsymbol{q}_i$ should have the same meaning as the position of the i-th particle coordinate $\boldsymbol{r}_i$ in the laboratory frame. Also the first Jacobi internal coordinate $\boldsymbol{\xi}_1$ should have the same meaning as the position of the first particle coordinate $\boldsymbol{r}_1$ because $\boldsymbol{\xi}_1 = (N/(N-1))\boldsymbol{q}_1 \to \boldsymbol{r}_1$ for $N \to \infty$.

As shown in Eqs. (30) and (31), the PP-type internal density matrix in the macroscopic limit does not satisfy the condition, while the density matrix of the Jacobi-type fulfills this condition as given in Eqs. (50) and (51). As already mentioned, the reason why the PP-type internal density matrix does not satisfy the physical boundary condition is due to the fact

that it exhibits a nonvanishing cross term or correlation term $\boldsymbol{q} \cdot \boldsymbol{q}'$ in the case of $N = \infty$, originating from the pseudo two-body interaction terms in the internal Hamiltonian. On the other hand, in the Jacobi-type internal density matrix, the pseudo two-body interaction terms disappear.

These results mean that one should take internal coordinates which do not produce any correlation in the internal one-particle density matrix in the macroscopic limit. Otherwise, unphysical situations occur like for the PP-type internal density matrix. One choice fulfilling the physical condition is the one of the internal Jacobi coordinates. Of course, there are many sets of internal coordinates which satisfy the physical condition. For example, they may be those satisfying the following two conditions: (1) The relative coordinate $\boldsymbol{\xi}$ between one particle and the other remaining particles should be used as the coordinate of the internal one-particle density matrix $\rho_{\mathrm{int}}^{(1)}$, and (2) the internal one-particle density matrix be separable with respect to $\boldsymbol{\xi}$ and $\boldsymbol{\xi}'$ in the macroscopic limit, $\rho_{\mathrm{int}}^{(1)}(\boldsymbol{\xi}, \boldsymbol{\xi}') \to (2\nu/\pi)^{3/2} \exp[-\nu(\boldsymbol{\xi}^2 + \boldsymbol{\xi}'^2)]$ for $N \to \infty$. Among the coordinates satisfying the two conditions, Jacobi coordinates are very convenient and useful to describe the internal Hamiltonian and thus the internal one-particle density matrix. We will see in the next section that this is in fact the only choice.

B. Orthogonality of the Coordinate $\boldsymbol{\xi}_1$ with respect to the $(N-2)$ Internal Coordinates

In the previous section, a criterion was discussed for the choice of the adequate coordinate systems of the internal density matrix. Here we present the other criterion that the coordinate of the internal one-body density matrix, $\boldsymbol{\xi}_1$, should be orthogonal to the remaining $(N-2)$ internal coordinates, where the $(N-2)$ coordinates do not need to be mutually orthogonal. This is called "maximal independence of the coordinate $\boldsymbol{\xi}_1$ from the rest of $(N-2)$ internal coordinates".

The coordinate of the internal one-particle density matrix should be either the one particle coordinate measured from the total center-of-mass or the one particle coordinate measured from the center-of-mass of the other $(N-1)$ particles. The PP-type internal one-particle density matrix adopts the former type coordinate $\boldsymbol{q}_1$ while the Jacobi-type internal one-particle density matrix adopts the latter type coordinate $\boldsymbol{\xi}_1$, coinciding in the macroscopic number. These two types of coordinates are essentially the same since they are related by

$\boldsymbol{q}_1 = ((N-1)/N)\boldsymbol{\xi}_1$. In constructing the internal one-particle density matrix, we integrate the internal density matrix over the other $(N-2)$ internal coordinates. In order for the internal one-particle density matrix to have maximum information on the one-particle degree-of-freedom of the system, these $(N-2)$ internal coordinates should be maximally independent from the coordinate $\boldsymbol{q}_1$ or $\boldsymbol{\xi}_1$. Since this requirement seems natural, we will study in this subsection its consequence. We will see below that this requirement implies the criterion proposed in the preceding subsection.

The requirement that the coordinate $\boldsymbol{q}_1$ or $\boldsymbol{\xi}_1$ is maximally independent from the other $(N-2)$ internal coordinates means mathematically that coordinate $\boldsymbol{q}_1$ or $\boldsymbol{\xi}_1$ should be orthogonal to the other $(N-2)$ internal coordinates. The Jacobi coordinates are just such coordinates, since they constitute an orthogonal coordinate system. On the other hand the internal coordinates $\{\boldsymbol{q}_i,\ i = 1 \sim (N-1)\}$ do not satisfy this requirement since they constitute a non-orthogonal coordinate system. For the sake of self-containedness we recall here the meaning of orthogonality between coordinates. Two coordinates $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ are defined to be mutually orthogonal when their expansion coefficients of linear combination with respect to the N particle coordinates $\{\boldsymbol{r}_i,\ (i = 1 \sim N)\}$, $\{C_i(\boldsymbol{\beta}),\ (i = 1 \sim N)\}$ and $\{C_i(\boldsymbol{\gamma}),\ (i = 1 \sim N)\}$,

$$\boldsymbol{\beta} = \sum_{i=1}^{N} C_i(\boldsymbol{\beta})\boldsymbol{r}_i, \quad \boldsymbol{\gamma} = \sum_{i=1}^{N} C_i(\boldsymbol{\gamma})\boldsymbol{r}_i, \tag{53}$$

are mutually orthogonal, $\sum_{i=1}^{N} C_i(\boldsymbol{\beta})C_i(\boldsymbol{\gamma}) = 0$. This definition can be stated as follows. To any coordinate $\boldsymbol{\delta}$ we associate an N-dimensional number vector $\boldsymbol{C}(\boldsymbol{\delta})$ like $\boldsymbol{C}(\boldsymbol{\beta}) = \{C_i(\boldsymbol{\beta}),\ (i = 1 \sim N)\}$ for $\boldsymbol{\beta}$ and $\boldsymbol{C}(\boldsymbol{\gamma}) = \{C_i(\boldsymbol{\gamma}),\ (i = 1 \sim N)\}$ for $\boldsymbol{\gamma}$. If $\boldsymbol{\beta} \neq \boldsymbol{\gamma}$, $\boldsymbol{C}(\boldsymbol{\beta}) \neq \boldsymbol{C}(\boldsymbol{\gamma})$. $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ are said to be orthogonal when $\boldsymbol{C}(\boldsymbol{\beta}) \cdot \boldsymbol{C}(\boldsymbol{\gamma}) = 0$. Needless to say, the total center-of-mass coordinate $\boldsymbol{R}$ is orthogonal to any kind of internal coordinates $\boldsymbol{\delta}_{\text{int}}$, i.e. $\boldsymbol{C}(\boldsymbol{R}) \cdot \boldsymbol{C}(\boldsymbol{\delta}_{\text{int}}) = 0$.

Let an internal coordinate system $\{\boldsymbol{\eta}_i,\ (i = 1 \sim (N-1))\}$ be such a system satisfying the above-mentioned requirement. The coordinate $\boldsymbol{\eta}_1$ is either $\boldsymbol{q}_1$ or $\boldsymbol{\xi}_1$ and hence we here fix it as $\boldsymbol{\eta}_1 = \boldsymbol{\xi}_1$. The orthogonality of $\boldsymbol{\xi}_1$ to the other $(N-2)$ coordinates $\{\boldsymbol{\eta}_i,\ (i = 2 \sim (N-1))\}$ means $\boldsymbol{C}(\boldsymbol{\xi}_1) \cdot \boldsymbol{C}(\boldsymbol{\eta}_i) = 0,\ (i = 2 \sim (N-1))$. Since the internal Jacobi coordinate system $\{\boldsymbol{\xi}_i,\ (i = 1 \sim (N-1))\}$ is an orthogonal coordinate system, there the relations $\boldsymbol{C}(\boldsymbol{\xi}_1) \cdot \boldsymbol{C}(\boldsymbol{\xi}_i) = 0,\ (i = 2 \sim (N-1))$ holds. Therefore the subspace spanned by the N-dimensional vectors $\{\boldsymbol{C}(\boldsymbol{\eta}_i),\ (i = 2 \sim (N-1))\}$ is identical to the subspace spanned

by N-dimensional vectors $\{C(\boldsymbol{\xi}_i),\ (i = 2 \sim (N-1))\}$. We, therefore, have

$$C(\boldsymbol{\xi}_i) = \sum_{j=2}^{N-1} d_{ij} C(\boldsymbol{\eta}_j),\ (i = 2 \sim (N-1)). \tag{54}$$

This relation is equivalent to the relation

$$\boldsymbol{\xi}_i = \sum_{j=2}^{N-1} d_{ij} \boldsymbol{\eta}_j,\ (i = 2 \sim (N-1)). \tag{55}$$

By inserting Eq. (55) into Eq. (42) we obtain

$$\sum_{i=1}^{N} \boldsymbol{r}_i^2 = N\boldsymbol{R}^2 + \sum_{i=1}^{N-1} \frac{\nu_i}{\nu} \boldsymbol{\xi}_i^2 \tag{56}$$

$$= N\boldsymbol{R}^2 + \frac{\nu_1}{\nu} \boldsymbol{\eta}_1^2 + \sum_{i,i'=2}^{N-1} a_{i,i'} \boldsymbol{\eta}_i \cdot \boldsymbol{\eta}_{i'}, \tag{57}$$

$$a_{i,i'} = \sum_{j=2}^{N-1} \frac{\nu_j}{\nu} d_{j,i} d_{j,i'}. \tag{58}$$

It is to be noticed that unlike the Jacobi coordinates the mutual orthogonality within the $(N-2)$ coordinates $\{\boldsymbol{\eta}_i,\ i = 2 \sim (N-1)\}$ does not hold in general.

By using Eq. (57) we can calculate the internal one-particle density matrix $\rho_{\mathrm{int}}^{(1)}$ as follows

$$\rho_{\mathrm{int}}^{(1)}(\boldsymbol{\eta}, \boldsymbol{\eta}') \propto \int d\boldsymbol{\eta}_2 \cdots d\boldsymbol{\eta}_{N-1} \exp\left[-\nu \left(\frac{\nu_1}{\nu} \boldsymbol{\eta}^2 + \sum_{i,i'=2}^{N-1} a_{i,i'} \boldsymbol{\eta}_i \cdot \boldsymbol{\eta}_{i'} \right) \right]$$

$$\times \exp\left[-\nu \left(\frac{\nu_1}{\nu} \boldsymbol{\eta}'^2 + \sum_{i,i'=2}^{N-1} a_{i,i'} \boldsymbol{\eta}_i \cdot \boldsymbol{\eta}_{i'} \right) \right] \tag{59}$$

$$\propto \exp\left[-\frac{N-1}{N} \nu \left(\boldsymbol{\eta}^2 + \boldsymbol{\eta}'^2 \right) \right]. \tag{60}$$

This result shows that $\rho_{\mathrm{int}}^{(1)}(\boldsymbol{\eta}, \boldsymbol{\eta}')$ is just the same as the Jacobi-type internal one-particle density matrix. Thus we see that our above requirement concerning the internal coordinates, gives us a *unique result* for the internal one-particle density matrix. It is just identical to the Jacobi-type internal one-particle density matrix.

In the previous section III A we have proposed also another requirement, namely that the internal one-particle density matrix should converge to the one-particle density matrix in the laboratory frame in the macroscopic limit. As we discussed in Sec. III A, this requirement implies that there should not appear any cross terms of $\boldsymbol{\xi}_1$ with the other internal coordinates in the internal wave function at least in the macroscopic limit. Clearly the absence of the cross terms of $\boldsymbol{\xi}_1$ with the other internal coordinates is realized only when the coordinate

$\boldsymbol{\xi}_1$ is orthogonal to all the other $(N-2)$ internal coordinates. Thus the criterion in the preceding subsection results from the present requirement of the orthogonality of $\boldsymbol{\xi}_1$ to the other $(N-2)$ internal coordinates, where the $(N-2)$ coordinates generally do not need to be mutually orthogonal.

One may argue that a physical quantity should not depend on the choice of the coordinate system. In the case of the one-particle density matrix this argument can be true under the condition that we have extracted maximum information on the one-particle degree of freedom of the system. As already noticed this condition is the same as the requirement that the coordinate of the one-particle density matrix is orthogonal to all the other coordinates of the system. This is also true in the macroscopic system where we usually adopt the coordinate system composed of individual particle coordinates $\{\boldsymbol{r}_i,\ (i = 1 \sim N)\}$. The coordinate $\boldsymbol{r}_1$ of the one-particle density matrix is of course orthogonal to all the other coordinates. If we adopt the coordinate system $\{\boldsymbol{R}, \boldsymbol{q}_i,\ (i = 1 \sim (N-1))\}$ and calculate the one-particle density matrix with respect to the coordinate $\boldsymbol{q}_1$ which is practically the same as $\boldsymbol{r}_1$ in the macroscopic system by integrating out the remaining coordinates $\{\boldsymbol{R}, \boldsymbol{q}_i,\ (i = 2 \sim (N-1))\}$, we get the result given in Eq. (29), namely $(2\nu/\pi)^{3/2} \exp[-(3/2)\nu(\boldsymbol{q}_1^2 + \boldsymbol{q}_1'^2) + \nu \boldsymbol{q}_1 \cdot \boldsymbol{q}_1']$. This inadequate result is, of course, due to the non-orthogonality of $\boldsymbol{q}_1$ to the other coordinates $\{\boldsymbol{q}_i,\ (i = 2 \sim (N-1))\}$, as we have already seen earlier.

The PP-type internal one-particle density matrix $\rho_{\mathrm{int,PP}}^{(1)}$ is different from the Jacobi-type one $\rho_{\mathrm{int,J}}^{(1)}$. This is true for the non-diagonal elements but for the diagonal elements they are the same except for the Jacobian factor $\partial(\boldsymbol{q}_1)/\partial(\boldsymbol{\xi}_1) = ((N-1)/N)^3$, (which goes to unity in the macroscopic limit)

$$\rho_{\mathrm{int,PP}}^{(1)}(\boldsymbol{q}_1, \boldsymbol{q}_1) = \left(\frac{N}{N-1}\right)^3 \rho_{\mathrm{int,J}}^{(1)}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_1). \tag{61}$$

It is to be noticed that both $\rho_{\mathrm{int,PP}}^{(1)}$ and $\rho_{\mathrm{int,J}}^{(1)}$ are normalized,

$$\int d\boldsymbol{q}_1 \rho_{\mathrm{int,PP}}^{(1)}(\boldsymbol{q}_1, \boldsymbol{q}_1) = \int d\boldsymbol{\xi}_1 \rho_{\mathrm{int,J}}^{(1)}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_1) = 1. \tag{62}$$

The equality of Eq. (61) is easily proved by using Eqs. (20) and (45). Let us study these relations between $\rho_{\mathrm{int,PP}}^{(1)}$ and $\rho_{\mathrm{int,J}}^{(1)}$ a little more in detail. First we note the relation between the two coordinate systems, $\{\boldsymbol{q}_i,\ (i = 1 \sim (N-1))\}$ and $\{\boldsymbol{\xi}_i,\ (i = 1 \sim (N-1))\}$,

$$\boldsymbol{q}_i = -\sum_{j=1}^{i-1} \frac{1}{N+1-j}\boldsymbol{\xi}_j + \frac{N-1}{N+1-i}\boldsymbol{\xi}_i. \tag{63}$$

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When we calculate $\rho_{\mathrm{int,J}}^{(1)}$, we make the following integration

$$\rho_{\mathrm{int,J}}^{(1)}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_1') = \int d\boldsymbol{\xi}_2 \cdots d\boldsymbol{\xi}_{N-1} \, \Phi_{\mathrm{int}}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})\Phi_{\mathrm{int}}(\boldsymbol{\xi}_1', \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1}) \tag{64}$$

$$= \frac{\partial(\boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})}{\partial(\boldsymbol{q}_2, \cdots, \boldsymbol{q}_{N-1})} \int d\boldsymbol{q}_2 \cdots d\boldsymbol{q}_{N-1} \, \widehat{\Phi}_{\mathrm{int}}(\boldsymbol{q}_1, \boldsymbol{q}_2, \cdots, \boldsymbol{q}_{N-1})$$

$$\times \widehat{\Phi}_{\mathrm{int}}(\boldsymbol{q}_1', \boldsymbol{q}_2', \cdots, \boldsymbol{q}_{N-1}') \tag{65}$$

$$\boldsymbol{q}_i' = \boldsymbol{q}_i(\boldsymbol{\xi}_1 \to \boldsymbol{\xi}_1') = \boldsymbol{q}_i + \frac{1}{N}(\boldsymbol{\xi}_1 - \boldsymbol{\xi}_1'), \tag{66}$$

where

$$\widehat{\Phi}_{\mathrm{int}}(\boldsymbol{q}_1, \boldsymbol{q}_2, \cdots, \boldsymbol{q}_{N-1}) = \Phi_{\mathrm{int}}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1}), \tag{67}$$

$$\widehat{\Phi}_{\mathrm{int}}(\boldsymbol{q}_1', \boldsymbol{q}_2', \cdots, \boldsymbol{q}_{N-1}') = \Phi_{\mathrm{int}}(\boldsymbol{\xi}_1', \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1}). \tag{68}$$

For non-diagonal elements of $\rho_{\mathrm{int,J}}^{(1)}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_1')$, since $\boldsymbol{\xi}_1 \neq \boldsymbol{\xi}_1'$, it follows that $\boldsymbol{q}_i' \neq \boldsymbol{q}_i$ for all $i = 1 \sim (N-1)$. This tells us that $\rho_{\mathrm{int,J}}^{(1)}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_1')$ can not be proportional to $\rho_{\mathrm{int,PP}}^{(1)}(\boldsymbol{q}_1, \boldsymbol{q}_1')$ because the latter is obtained from

$$\int d\boldsymbol{q}_2 \cdots d\boldsymbol{q}_{N-1} \, \widehat{\Phi}_{\mathrm{int}}(\boldsymbol{q}_1, \boldsymbol{q}_2, \cdots, \boldsymbol{q}_{N-1}) \, \widehat{\Phi}_{\mathrm{int}}(\boldsymbol{q}_1', \boldsymbol{q}_2, \cdots, \boldsymbol{q}_{N-1}). \tag{69}$$

On the other hand, for diagonal elements, $\rho_{\mathrm{int,J}}^{(1)}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_1)$, since $\boldsymbol{\xi}_1 = \boldsymbol{\xi}_1'$, there follows $\boldsymbol{q}_i' = \boldsymbol{q}_i$ for all $i = 1 \sim (N-1)$. This tells us that $\rho_{\mathrm{int,J}}^{(1)}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_1)$ is now proportional to $\rho_{\mathrm{int,PP}}^{(1)}(\boldsymbol{q}_1, \boldsymbol{q}_1)$. The appearance of the term $(1/N)(\boldsymbol{\xi}_1 - \boldsymbol{\xi}_1')$ in the relation $\boldsymbol{q}_i' = \boldsymbol{q}_i + (1/N)(\boldsymbol{\xi}_1 - \boldsymbol{\xi}_1')$ just stems from the non-orthogonality of $\boldsymbol{q}_1$ to $\boldsymbol{q}_i$ ($i = 2 \sim (N-1)$).

We have proved in this section that the internal one-body density matrix is uniquely determined for the $0S$ harmonic oscillator wave function. However, it is noted that this uniqueness holds in the case of a general wave function including the $0S$ harmonic oscillator one. In fact, Suzuki et al. [29, 30] have already given the proof of the uniqueness for the more general wave function Ψ which is expanded in terms of the correlated Gaussian basis g. The explicit forms of Ψ and g are expressed as follows:

$$\Psi = \sum_k C_k \mathcal{S} g(\boldsymbol{s}^{(k)}; A^{(k)}, \boldsymbol{x}) \tag{70}$$

$$g = g(\boldsymbol{s}; A, \boldsymbol{x}) = \exp\left[-\frac{1}{2}\sum_{i,j} A_{ij}\boldsymbol{x}_i \cdot \boldsymbol{x}_j + \sum_i \boldsymbol{s}_i \cdot \boldsymbol{x}_i \right], \tag{71}$$

where $\boldsymbol{x} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_{N-1}\}$ and $\mathcal{S}$ are a set of internal coordinate of N-boson system and the symmetrization operator acting on the N bosons, respectively. C_k, $A^{(k)}$ and $\boldsymbol{s}^{(k)}$ are the

expansion parameters, in which $A^{(k)}$ denotes a symmetric positive-defined $(N-1) \times (N-1)$ matrix, and $\boldsymbol{s}^{(k)}$ represents $\boldsymbol{s}^{(k)} = \{\boldsymbol{s}_1^{(k)}, \boldsymbol{s}_2^{(k)}, \cdots, \boldsymbol{s}_{N-1}^{(k)}\}$. The correlated Gaussian basis g is often used in ab-initio calculations and has succeeded in describing structures of many few-body systems [31]. The uniqueness of the internal one-body density matrix ρ for the wave function Ψ in Eq. (70) is proved [29, 30] under the condition that one takes the following set of coordinates $\boldsymbol{y} = \{\boldsymbol{y}_1, \boldsymbol{y}_2, \cdots, \boldsymbol{y}_{N-1}\}$ (obtained by a linear transformation from the coordinates $\boldsymbol{x}$) as the coordinates of Ψ adopted in calculating ρ: $\boldsymbol{q}_1$ is chosen as the coordinate $(\boldsymbol{y_1})$ of the internal one-body density matrix and the remaining $(N-2)$ internal coordinates $(\boldsymbol{y}_2, \boldsymbol{y}_3, \cdots, \boldsymbol{y}_{N-1})$ are orthogonal to $\boldsymbol{q}_1$, although the $(N-2)$ coordinates do not need to be mutually orthogonal. This requirement for the coordinates $\boldsymbol{y}$ just corresponds to the "maximally independence of the coordinate $\boldsymbol{\xi}_1$ $(\boldsymbol{q}_1)$ from the rest of $(N-2)$ internal coordinates" as mentioned above. The proof we gave in this section is specified to the simple system which is composed of N bosons in the harmonic oscillator potential and has been discussed by many authors (for example, see Refs. [18, 19, 21, 22]).

IV. SUMMARY

We investigated the internal one-particle density matrix in the case of ideal Bose-Einstein condensates with a finite number (N) of particles in a harmonic trap. We calculated the explicit form of the internal one-particle density matrix following the definition of Pethick and Pitaevskii (PP) and solved its eigenvalue problem. The result was found to show a fragmented condensate, contrary to what PP expected. On the other hand the Jacobi-type internal one-particle density matrix gives us complete condensation. It means that the internal one-particle density matrix is different in general for different choices of the internal coordinate system. In this paper we outlined two physically motivated criteria for the choice of the adequate coordinate system leading to a unique answer for the internal one-particle density matrix. One criterion is that in the infinite particle number ($N = \infty$) limit the internal one-particle density matrix should have the same eigenvalues and eigenfunctions as those of the corresponding ideal Bose-Einstein condensate in the laboratory frame. The other criterion is that the coordinate of the internal one-particle density matrix which is either $\boldsymbol{q}_1 = \boldsymbol{r}_1 - \boldsymbol{R}$ or $\boldsymbol{\xi}_1 = (N/(N-1))\boldsymbol{q}_1$, should be maximally independent from the remaining $(N-2)$ internal coordinates. Mathematically this criterion means that $\boldsymbol{q}_1$ (or $\boldsymbol{\xi}_1$)

is orthogonal to the remaining $(N-2)$ internal coordinates, though the $(N-2)$ coordinates, in general, do not need to be mutually orthogonal. This second criterion was shown to imply the first criterion. We saw that the internal Jacobi coordinate system satisfies these two criteria while the internal coordinate system adopted by Pethick and Pitaevskii for the construction of the internal one-particle density matrix does not. Furthermore we argued that these two criteria *uniquely* determine the internal one-particle density matrix which is the same as that calculated with the Jacobi coordinates. The results of this paper justify the use of the Jacobi coordinates in Refs. [16, 17] where the Bose condensation of a few α-particles in extended states of self-conjugate light nuclei was considered. However, our results are of more general interest. For example the number of bosons captured in each site of an optical lattice is often very small [28] and, therefore, our analysis surely applies to that situation as well. We also believe that our present study has considerably clarified the somewhat controversial issue of how to define a Bose condensate of a finite number of particles in their internal coordinate system. This question is particularly, but not only, relevant for selfbound Bose systems, like a loosely bound gas of α-particles in nuclei or nano-droplets of liquid ^{4}He.

APPENDIX A: SOLUTION OF THE EIGENVALUE PROBLEM OF THE SYMMETRIC GAUSSIAN INTEGRAL KERNEL

The one-particle density matrices discussed in this paper are symmetric Gaussian integral kernels of the form

$$\langle \boldsymbol{r}|\hat{Q}|\boldsymbol{r}'\rangle = Q(\boldsymbol{r},\boldsymbol{r}') = \left(\frac{2a-b}{\pi}\right)^{\frac{3}{2}} \exp\{-a(\boldsymbol{r}^2+\boldsymbol{r}'^2)+b\boldsymbol{r}\cdot\boldsymbol{r}'\}. \tag{A1}$$

This kernel is normalized

$$\text{Tr}\,\hat{Q} = \int d\boldsymbol{r}\,Q(\boldsymbol{r},\boldsymbol{r}) = 1, \tag{A2}$$

for which we need the condition $2a-b>0$.

The eigenvalue problem of the kernel $Q(\boldsymbol{r}, \boldsymbol{r}')$ can be solved analytically. There are several ways to solve it. We can e.g. use the method given in Ref. [27]. Here we explain another procedure which gives us the following answer (see below)

$$\hat{Q} = \left(\frac{2a-b}{a+c}\right)^{\frac{3}{2}} \left(\frac{2(a-c)}{b}\right)^{\boldsymbol{\alpha}_c^\dagger \cdot \boldsymbol{\alpha}_c}, \quad c = \sqrt{a^2 - \frac{b^2}{4}}, \tag{A3}$$

$$\boldsymbol{\alpha}_c^\dagger = \sqrt{c}\left(\boldsymbol{r} - \frac{1}{2c}\frac{\partial}{\partial\boldsymbol{r}}\right), \quad \boldsymbol{\alpha}_c = \sqrt{c}\left(\boldsymbol{r} + \frac{1}{2c}\frac{\partial}{\partial\boldsymbol{r}}\right). \tag{A4}$$

Here $\boldsymbol{\alpha}_c^\dagger$ and $\boldsymbol{\alpha}_c$ are creation and annihilation operators of harmonic oscillation of size parameter c, respectively. The eigenfunctions of $\hat{Q}$ are just the same as those of the operator $\boldsymbol{\alpha}_c^\dagger \cdot \boldsymbol{\alpha}_c$ which are of course the harmonic oscillator functions of the size parameter c. Thus we have

$$\hat{Q}|\phi_{nLM}(c)\rangle = \lambda_n^{(L,M)}|\phi_{nLM}(c)\rangle, \tag{A5}$$

$$\langle\boldsymbol{r}|\phi_{nLM}(c)\rangle = \phi_{nLM}(\boldsymbol{r}, c), \tag{A6}$$

$$\lambda_n^{(L,M)} = \left(\frac{2a-b}{a+c}\right)^{\frac{3}{2}} \left(\frac{2(a-c)}{b}\right)^{2n+L}. \tag{A7}$$

The explicit form of $\phi_{nLM}(\boldsymbol{r}, c)$ is given in Eq. (23). It is to be noted that the eigenvalue $\lambda_n^{(L,M)}$ depends only on the number of harmonic oscillator quanta $(2n + L)$. It is just the SU(3)-scalar property of the operator $\hat{Q}$. A merit of our method as explained below, is that it gives us a clearer understanding of the SU(3) symmetry of the operator $\hat{Q}$.

The relation of Eq. (A3) comes directly from the following theorem [32] valid for a general operator P:

$$P = \mathcal{N}_{\mathrm{op}}\{p(\boldsymbol{\alpha}_\gamma^\dagger, \boldsymbol{\alpha}_\gamma)\}, \tag{A8}$$

where $\mathcal{N}_{\mathrm{op}}$ is the operator of normal ordering, and

$$\boldsymbol{\alpha}_\gamma^\dagger = \sqrt{\gamma}\left(\boldsymbol{r} - \frac{1}{2\gamma}\frac{\partial}{\partial\boldsymbol{r}}\right), \quad \boldsymbol{\alpha}_\gamma = \sqrt{\gamma}\left(\boldsymbol{r} + \frac{1}{2\gamma}\frac{\partial}{\partial\boldsymbol{r}}\right), \tag{A9}$$

$$p(\boldsymbol{Z}^*, \boldsymbol{Z}) = \frac{\langle A_\gamma(\boldsymbol{Z})|P|A_\gamma(\boldsymbol{Z}')\rangle}{\langle A_\gamma(\boldsymbol{Z})|A_\gamma(\boldsymbol{Z}')\rangle} \tag{A10}$$

$$= \exp(-\boldsymbol{Z}^* \cdot \boldsymbol{Z}')\langle A_\gamma(\boldsymbol{Z})|P|A_\gamma(\boldsymbol{Z}')\rangle, \tag{A11}$$

$$\langle\boldsymbol{r}|A_\gamma(\boldsymbol{Z})\rangle = A_\gamma(\boldsymbol{r}, \boldsymbol{Z}) = \left(\frac{2\gamma}{\pi}\right)^{\frac{3}{4}} \exp\left[-\gamma\left(\boldsymbol{r} - \frac{\boldsymbol{Z}}{\sqrt{\gamma}}\right)^2 + \frac{1}{2}\boldsymbol{Z}^2\right]. \tag{A12}$$

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The state $|A_\gamma(\boldsymbol{Z})\rangle$ is the well-known coherent state of harmonic oscillator of size parameter γ,

$$|A_\gamma(\boldsymbol{Z})\rangle = \exp\{\boldsymbol{Z} \cdot \boldsymbol{\alpha}_\gamma^\dagger\} \, |A_\gamma(\boldsymbol{Z} = 0)\rangle, \tag{A13}$$

$$\boldsymbol{\alpha}_\gamma |A_\gamma(\boldsymbol{Z})\rangle = \boldsymbol{Z}|A_\gamma(\boldsymbol{Z})\rangle, \tag{A14}$$

$$A_\gamma(\boldsymbol{r}, \boldsymbol{Z}) = A_\gamma(x, Z_x)A_\gamma(y, Z_y)A_\gamma(z, Z_z), \tag{A15}$$

$$A_\gamma(x, Z_x) = \left(\frac{2\gamma}{\pi}\right)^{\frac{1}{4}} \exp\left[-\gamma\left(x - \frac{Z_x}{\sqrt{\gamma}}\right)^2 + \frac{1}{2}Z_x^2\right] \tag{A16}$$

$$= \sum_{n=0}^\infty \frac{(Z_x)^n}{\sqrt{n!}} X_n(x, \gamma), \tag{A17}$$

$$X_n(x, \gamma) = \frac{(\alpha_{\gamma,x}^\dagger)^n}{\sqrt{n!}} A_\gamma(x, Z_x = 0). \tag{A18}$$

The proof of the general theorem of Eq. (A8) is quite easy. It is given by comparing the matrix elements of two operators, P and $\mathcal{N}_{\text{op}}\{p(\boldsymbol{\alpha}_\gamma^\dagger, \boldsymbol{\alpha}_\gamma)\}$, formed with the coherent states $|A_\gamma(\boldsymbol{Z})\rangle$ which constitute an overcomplete set of states. This is shown by the following operation:

$$\langle A_\gamma(\boldsymbol{Z})|\mathcal{N}_{\text{op}}\{p(\boldsymbol{\alpha}_\gamma^\dagger, \boldsymbol{\alpha}_\gamma)\}|A_\gamma(\boldsymbol{Z}')\rangle = p(\boldsymbol{Z}^*, \boldsymbol{Z}')\langle A_\gamma(\boldsymbol{Z})|A_\gamma(\boldsymbol{Z}')\rangle \tag{A19}$$

$$= \langle A_\gamma(\boldsymbol{Z})|P|A_\gamma(\boldsymbol{Z}')\rangle. \tag{A20}$$

The equality of Eq. (A19) is due to Eq. (A14).

By applying the above general theorem to our present operator Q of Eq. (A1), we obtain

$$q(\boldsymbol{Z}^*, \boldsymbol{Z}) = \frac{\langle A_\gamma(\boldsymbol{Z})|Q|A_\gamma(\boldsymbol{Z}')\rangle}{\langle A_\gamma(\boldsymbol{Z})|A_\gamma(\boldsymbol{Z}')\rangle} \tag{A21}$$

$$= \left(\frac{\pi^2}{(\gamma + a)^2 - (b^2/4)}\right)^{\frac{3}{2}} \exp\left[F(\boldsymbol{Z}^{*2} + \boldsymbol{Z}'^2) + G\boldsymbol{Z}^* \cdot \boldsymbol{Z}'\right], \tag{A22}$$

$$F = -\frac{1}{2} + \frac{\gamma(\gamma + a)}{(\gamma + a)^2 - (b^2/4)}, \tag{A23}$$

$$G = -1 + \frac{\gamma b}{(\gamma + a)^2 - (b^2/4)}. \tag{A24}$$

By choosing

$$\gamma = c = \sqrt{a^2 - \frac{b^2}{4}}, \tag{A25}$$

we obtain $F = 0$. Thus we have for $\gamma = c$

$$q(\boldsymbol{Z}^*, \boldsymbol{Z}') = \left(\frac{2a - b}{a + c}\right)^{\frac{3}{2}} \exp\left[\left(\frac{2(a - c)}{b} - 1\right)\boldsymbol{Z}^* \cdot \boldsymbol{Z}'\right]. \tag{A26}$$

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By using the well-known formula [33]

$$\mathcal{N}_{\mathrm{op}}\{\exp[(Y-1)\boldsymbol{\alpha}_\gamma^\dagger \cdot \boldsymbol{\alpha}_\gamma]\} = Y^{\boldsymbol{\alpha}_\gamma^\dagger \cdot \boldsymbol{\alpha}_\gamma}, \tag{A27}$$

we obtain the desired result of Eq. (A3)

$$Q = \mathcal{N}_{\mathrm{op}}\{q(\boldsymbol{\alpha}_c^\dagger, \boldsymbol{\alpha}_c)\} \tag{A28}$$

$$= \left(\frac{2a-b}{a+c}\right)^{\frac{3}{2}} \left(\frac{2(a-c)}{b}\right)^{\boldsymbol{\alpha}_c^\dagger \cdot \boldsymbol{\alpha}_c}. \tag{A29}$$

The formula of Eq. (A27) can also easily be proved by comparing the matrix elements of $\mathcal{N}_{\mathrm{op}}\{\exp[(Y-1)\boldsymbol{\alpha}_\gamma^\dagger \cdot \boldsymbol{\alpha}_\gamma]\}$ and $Y^{\boldsymbol{\alpha}_\gamma^\dagger \cdot \boldsymbol{\alpha}_\gamma}$ formed with coherent states. For treating $Y^{\boldsymbol{\alpha}_\gamma^\dagger \cdot \boldsymbol{\alpha}_\gamma}$, the expansion of the coherent state by harmonic oscillator functions given in Eq. (A17) is useful.

APPENDIX B: BOSONIC SYMMETRY OF THE JACOBI-TYPE INTERNAL ONE-PARTICLE DENSITY MATRIX

The bosonic symmetry of the Jacobi-type internal one-particle density matrix defined in Eq. (44) can be seen in the following identity relation,

$$\rho_{\mathrm{int,J}}^{(1)}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \int d\boldsymbol{\xi}_2 \cdots d\boldsymbol{\xi}_{N-1}\ \Phi_{\mathrm{int}}(\boldsymbol{\xi}, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})\Phi_{\mathrm{int}}(\boldsymbol{\xi}', \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1}) \tag{B1}$$

$$= \int d\boldsymbol{\xi}_1 d\boldsymbol{\xi}_2 \cdots d\boldsymbol{\xi}_{N-1} \times d\boldsymbol{\xi}_1' d\boldsymbol{\xi}_2' \cdots d\boldsymbol{\xi}_{N-1}'$$

$$\times \Phi_{\mathrm{int}}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})\widehat{O}(1, \boldsymbol{\xi}, \boldsymbol{\xi}')\Phi_{\mathrm{int}}(\boldsymbol{\xi}_1', \boldsymbol{\xi}_2', \cdots, \boldsymbol{\xi}_{N-1}') \tag{B2}$$

$$= \int d\boldsymbol{\xi}_1 d\boldsymbol{\xi}_2 \cdots d\boldsymbol{\xi}_{N-1} \times d\boldsymbol{\xi}_1' d\boldsymbol{\xi}_2' \cdots d\boldsymbol{\xi}_{N-1}'$$

$$\times \Phi_{\mathrm{int}}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})\frac{1}{N}\sum_{k=1}^{N}\widehat{O}(k, \boldsymbol{\xi}, \boldsymbol{\xi}')\Phi_{\mathrm{int}}(\boldsymbol{\xi}_1', \boldsymbol{\xi}_2', \cdots, \boldsymbol{\xi}_{N-1}'), \tag{B3}$$

$$\widehat{O}(k, \boldsymbol{\xi}, \boldsymbol{\xi}') = \delta(\boldsymbol{\xi}_1^k - \boldsymbol{\xi})\delta(\boldsymbol{\xi}_1^{k'} - \boldsymbol{\xi}')\prod_{j \geq 2}\delta(\boldsymbol{\xi}_j^k - \boldsymbol{\xi}_j^{k'}). \tag{B4}$$

Here we define N different sets of Jacobi coordinates $(\boldsymbol{\xi}_1^k, \boldsymbol{\xi}_2^k, \cdots, \boldsymbol{\xi}_{N-1}^k)$ by N cyclic permutations of particle indices $(1, 2, \cdots, N)$

$$\boldsymbol{\xi}_i^k = \boldsymbol{r}_{p_k(i)} - \frac{1}{N-i}\sum_{j=i+1}^{N}\boldsymbol{r}_{p_k(j)}, \tag{B5}$$

$$(p_k(1), p_k(2), \cdots, p_k(N)) = (k, k+1, \cdots, N, 1, 2, \cdots, k-1), \qquad (k = 1 \sim N). \tag{B6}$$

We should note that, since $\Phi_{\rm int}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})$ is totally symmetric for particle permutations as is clear from the relation $\Phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots, \boldsymbol{r}_N) = \Phi_{\rm int}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})\Phi_{\rm cm}(\boldsymbol{R})$, we have

$$\Phi_{\rm int}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1}) = \Phi_{\rm int}(\boldsymbol{\xi}_1^k, \boldsymbol{\xi}_2^k, \cdots, \boldsymbol{\xi}_{N-1}^k) \qquad (k = 1 \sim N). \tag{B7}$$

And of course we have

$$d\boldsymbol{\xi}_1 d\boldsymbol{\xi}_2 \cdots d\boldsymbol{\xi}_{N-1} = d\boldsymbol{\xi}_1^k d\boldsymbol{\xi}_2^k \cdots d\boldsymbol{\xi}_{N-1}^k. \tag{B8}$$

The expression of Eq. (B3) is the manifestation of the bosonic symmetry of the Jacobi-type internal one-particle density matrix. This equality is due to the following relations

$$\langle \widehat{O}(k, \boldsymbol{\xi}, \boldsymbol{\xi}') \rangle = \langle \widehat{O}(1, \boldsymbol{\xi}, \boldsymbol{\xi}') \rangle, \quad (k = 2 \sim N),, \tag{B9}$$

where $\langle \widehat{O}(k, \boldsymbol{\xi}, \boldsymbol{\xi}') \rangle$ is defined as

$$\begin{aligned} \langle \widehat{O}(k, \boldsymbol{\xi}, \boldsymbol{\xi}') \rangle &= \int d\boldsymbol{\xi}_1 d\boldsymbol{\xi}_2 \cdots d\boldsymbol{\xi}_{N-1} \times d\boldsymbol{\xi}'_1 d\boldsymbol{\xi}'_2 \cdots d\boldsymbol{\xi}'_{N-1} \\ &\times \Phi_{\rm int}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})\widehat{O}(k, \boldsymbol{\xi}, \boldsymbol{\xi}')\Phi_{\rm int}(\boldsymbol{\xi}'_1, \boldsymbol{\xi}'_2, \cdots, \boldsymbol{\xi}'_{N-1}), \\ &(k = 1 \sim N). \end{aligned} \tag{B10}$$

We can prove the equality of Eq. (B9), by using Eq. (B7) and Eq. (B8), as follows

$$\begin{aligned} \langle \widehat{O}(k, \boldsymbol{\xi}, \boldsymbol{\xi}') \rangle &= \int d\boldsymbol{\xi}_1 d\boldsymbol{\xi}_2 \cdots d\boldsymbol{\xi}_{N-1} \times d\boldsymbol{\xi}'_1 d\boldsymbol{\xi}'_2 \cdots d\boldsymbol{\xi}'_{N-1} \\ &\times \Phi_{\rm int}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})\widehat{O}(k, \boldsymbol{\xi}, \boldsymbol{\xi}')\Phi_{\rm int}(\boldsymbol{\xi}'_1, \boldsymbol{\xi}'_2, \cdots, \boldsymbol{\xi}'_{N-1}) \tag{B11} \\ &= \int d\boldsymbol{\xi}_1^k d\boldsymbol{\xi}_2^k \cdots d\boldsymbol{\xi}_{N-1}^k \times d\boldsymbol{\xi}_1^{k'} d\boldsymbol{\xi}_2^{k'} \cdots d\boldsymbol{\xi}_{N-1}^{k'} \\ &\times \Phi_{\rm int}(\boldsymbol{\xi}_1^k, \boldsymbol{\xi}_2^k, \cdots, \boldsymbol{\xi}_{N-1}^k)\widehat{O}(k, \boldsymbol{\xi}, \boldsymbol{\xi}')\Phi_{\rm int}(\boldsymbol{\xi}_1^{k'}, \boldsymbol{\xi}_2^{k'}, \cdots, \boldsymbol{\xi}_{N-1}^{k'}) \tag{B12} \\ &= \int d\boldsymbol{\xi}_1 d\boldsymbol{\xi}_2 \cdots d\boldsymbol{\xi}_{N-1} \times d\boldsymbol{\xi}'_1 d\boldsymbol{\xi}'_2 \cdots d\boldsymbol{\xi}'_{N-1} \\ &\times \Phi_{\rm int}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \cdots, \boldsymbol{\xi}_{N-1})\widehat{O}(1, \boldsymbol{\xi}, \boldsymbol{\xi}')\Phi_{\rm int}(\boldsymbol{\xi}'_1, \boldsymbol{\xi}'_2, \cdots, \boldsymbol{\xi}'_{N-1}) \tag{B13} \\ &= \langle \widehat{O}(1, \boldsymbol{\xi}, \boldsymbol{\xi}') \rangle. \tag{B14} \end{aligned}$$

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